Analysis of CO_2 Mass Transfer in Ionic Liquid–Water Mixtures by Thermophysical and Taylor Bubble Studies

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Understanding the multiscale mechanisms governing CO_2 absorption in ionic liquid (IL) based solvent systems is essential for the development of next-generation separation technologies. The behavior of these solvents emerges from different and interconnected phenomena: molecular interactions define thermophysical properties, such as viscosity and diffusivity, which in turn shape fluid dynamics and ultimately control gas–liquid mass transfer in contactors. In this work, we investigate this chain of dependencies for aqueous mixtures of 1-ethyl-3-methylimidazolium acetate (EMIM OAc) and 1-butyl-3-methylimidazolium tetrafluoroborate (BMIM BF_4), two hydrophilic ionic liquids that have gained significant attention for CO_2 capture [1].

A comprehensive dataset of viscosity, density, surface tension and electrical conductivity was collected for different IL–water compositions, both before and after CO_2 absorption. This allows us to quantify not only how CO_2 uptake alters the liquid microstructure, but also to understand the intricate correlations between composition, intermolecular interactions and macroscopic transport behavior. These measurements aim to help connect the molecular scale to the mass-transfer performance.

To assess the impact of these property changes on gas–liquid mass transfer, CO_2 absorption of Taylor bubbles in vertical capillaries of circular shape with varying but defined hydraulic diameters is studied. In this configuration, single Taylor bubbles are held stationary while high-speed imaging captures the evolution of the bubble volume, allowing the measurement of the CO2 uptake by the liquid phase. From the transient development of the bubble volume, liquid-side mass transfer coefficients k_L are extracted following established methodologies as described [2, 3, 4].

The combined thermophysical and Taylor bubble analysis highlights a strong coupling between solvent composition, CO_2-induced structuring and mass transport performance. Increasing IL content leads to higher viscosity and lower diffusivity, and the viscosity further increases upon CO_2 absorption. These effects translate into measurable shifts in the mass transfer coefficient k_L, demonstrating how subtle molecular reorganizations propagate across scales to influence macroscopic mass transfer.

Overall, the results provide new insight into the dynamic behavior of ionic liquid–water mixtures under CO_2 absorption conditions and support the rational design for larger scale ILs based gas–liquid contactors, including bubble column processes. This multiscale framework represents a step toward predictive and optimized formulations for energy efficient carbon-capture technologies.

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